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Theoretical Study of the Wanzlick Equilibrium

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Abstract

A theoretical study of the tetraaminoethylene–diaminocarbene dissociation reaction shows that equilibrium is more readily attained for benzimidazol-2-ylidenes and doubly bridged imidazol-2-ylidenes. For imidazolin-2-ylidenes, the ‘Wanzlick equilibrium’ is less likely to occur due to the high reaction barrier. We demonstrate that the equilibrium reaction can be catalyzed by an electrophile.